TENSOR NETWORKS AND THE ENUMERATION OF REGULAR SUBGRAPHS

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Abstract. We propose a universal approach to a range of enumeration problems in graphs. The key point is in contracting suitably chosen symmetric tensors placed at the vertices of a graph along the edges. In particular, this leads to an algorithm that counts the number of d-regular subgraphs of an arbitrary graph including the number of d-factors (previously we considered the case $d = 2$ with a special emphasis on the enumeration of Hamiltonian cycles; cf. math.CO/0403339). We briefly discuss the problem of the computational complexity of this algorithm.

1. Introduction

A *tensor network* is a collection of tensors placed at the vertices of a connected finite graph. The valency of each tensor must coincide with the degree of the corresponding vertex, and tensor indices are labelled by the half-edges incident to this vertex. Two tensors placed at adjacent vertices can be contracted over the pair of indices labelling the two half-edges of the connecting edge. This yields a tensor network with one tensor less than the original one (the underlying graph obtained by contracting the corresponding edge has also one vertex and one edge less). When contracting a loop, the tensor at its single vertex gets contracted over a pair of indices, and the total number of tensors (or vertices) remains unchanged. The total contraction along all edges of the graph gives a number (the graph reduces then to a single vertex with no edges).

The idea of placing tensors at vertices of graphs and contracting them along the edges traces back to Sylvester [5][1], who used this construction for obtaining polynomial invariants of symmetric tensors. Much later Penrose [3] reversed this idea to computing graph invariants (like the number of 3-edge colorings of a planar 3-regular graph) in his novel (though not quite successful) approach to the 4-color problem. Later

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[1]We owe this reference to A. A. Kirillov, Jr.

a number of other remarkable applications was found, first of all in the theory of Vassiliev knot invariants(see, e. g., [1]). Recently tensor network contraction was used to simulate quantum computation (cf. [2] and references therein).

Here we deal with contracting networks of specially chosen symmetric tensors. The result of contraction gives a generating function for the numbers of regular subgraphs of any type. In its simplest version this algorithm produces the number of factors of any given degree. We also comment on the computational complexity of this agorithm.

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2. Networks of symmetric tensors and graph functions

Let G be a finite graph (possibly with loops and multiple edges). The set of vertices of G we denote by $V(G) = \{v_1, \dots, v_n\}$, where $n = |V(G)|$ is the total number of vertices, and the set of edges of G we denote by $E(G)$. For each vertex v_i we denote by d_i its degree (or valency), $i = 1, \dots, n$. Then the number of edges of G is given by

$$|E(G)| = \frac{1}{2}\sum_{i=1}^{n} d_i.$$

Now let $\mathbb{F}$ be a field, and let $V \cong \mathbb{F}^r$ be a vector space of dimension r over $\mathbb{F}$. Fix a symmetric bilinear form $B : V \otimes V \longrightarrow \mathbb{F}$. The graph G together with the bilinear form B define a multilinear form

$$B_G : V^{\otimes d_1} \otimes \dots \otimes V^{\otimes d_n} \longrightarrow \mathbb{F}, \tag{1}$$

which is constructed as follows. At each vertex v_i of G we place d_i-th tensor power $V^{\otimes d_i}$ of the vector space V, where the factors are labeled by the half-edges of G incident to v_i. Each edge of G defines a contraction of two copies of V (corresponding to its two half-edges) by means of the bilinear form B. We obtain the multilinear form B_G by performing such contractions over the set $E(G)$ of all edges of G. Rigorously speaking, the multilinear form B_G depends on the order of half-edges at each vertex v_i, or, equvalently, on the order of factors in the tensor power $V^{\otimes d_i}$. However, its restriction to $S^{d_1}V \otimes \dots \otimes S^{d_n}V$, where S^dV denotes the d-th symmetric power of V, is defined uniquely.

Now fix a sequence $\mathcal{A} = \{A_1, A_2, \dots\}$ of symmetric contravariant d-valent tensors $A_d \in S^dV \subset V^{\otimes d}$. Here we consider tensor networks given by the triple $\{G, \mathcal{A}, B\}$. We treat the tensor product $A_{d_1} \otimes \dots \otimes A_{d_n}$ as an element of $V^{\otimes d_1} \otimes \dots \otimes V^{\otimes d_n}$ and consider the element

$$\mathcal{F}_{\mathcal{A},\,B}(G) = B_G(A_{d_1} \otimes \dots \otimes A_{d_i}) \in \mathbb{F}. \tag{2}$$

In other words, $\mathcal{F}_{\mathcal{A},B}(G)$ is the result of contracting the tensor network $\{G, \mathcal{A}, B\}$ – it is obtained by placing a copy of A_d at each vertex of G of degree d and contracting $\otimes_{i=1}^{n} A_{d_i}$ using B over $|E(G)|$ pairs of indices corresponding to the edges of G. Thus, to each pair $\mathcal{A}$, B, where $\mathcal{A}$ is a sequence of symmetric d-tensors ($d = 1, 2, \dots$) and B is a symmetric bilinear form, we associate an $\mathbb{F}$-valued mapping $\mathcal{F}_{\mathcal{A},B}$ on the set of isomorphism classes of graphs, or an $\mathbb{F}$-valued *graph function* in the terminology of [6].

3. Enumeration of regular subgraphs

Given a graph G, let H be a k-regular subgraph of G (not necessarily connected). The *type* of the subgraph H in G is the partition $\lambda_H = [|V(H_1)|, \dots, |V(H_l)|]$ of the number $|V(H)|$ of vertices of H, where $H_1, \dots, H_l$ are the connected componets of H, $l = l(H)$. The weight of partition λ_H is $|\lambda_H| = |V(H)|$, and the length is $l(\lambda_H) = l(H)$. For each partition λ we define a graph function $N_{k,\lambda}$ by

$$N_{k,\lambda}(G) = \#\{H \subset G | H \text{ is } k\text{-regular and } \lambda_H = \lambda\},$$

i.e., $N_{k,\lambda}(G)$ is the number of k-regular subgraphs of type λ in G. Clearly, $N_{k,\lambda}(G) = 0$ if $k > \max\{d_1, \dots, d_n\}$ or $|\lambda| > n$.

For k a positive integer, denote by $p_k(x_1, x_2, \dots) = x_1^k + x_2^k + \dots$ the k-th power sum in variables $x_1, x_2, \dots$. Given a partition $\lambda = [k_1, \dots, k_l]$, we define a homogeneous symmetric function p_λ of degree $|\lambda| = k_1 + \dots + k_l$ by the formula

$$p_\lambda(x_1, x_2, \dots) = \prod_{i=1}^{l} p_{k_i}(x_1, x_2, \dots).$$

We want to show that under a special choice of $\mathcal{A}$ and B the graph function $\mathcal{F}_{\mathcal{A},B}$ defined in Section 2 counts the number of k-regular subgraphs of any given type in graphs. We take $\mathbb{F} = \mathbb{C}$ and consider the standard coordinates in $V = \mathbb{C}^r$. In these coordinates the bilinear form B is given by the identity $r \times r$ matrix I_r. We define the tensors $A_{d,k}$ componentwise. For $d < k$ we put

$$A_{d,k}^{i_1 \dots i_d} = \begin{cases} 0 & \text{if } (i_1 \dots i_d) \neq (r \dots r), \\ t & \text{if } (i_1 \dots i_d) = (r \dots r), \end{cases}$$

and for $d \geq k$ we put

$$A_{d,k}^{i_1 \dots i_d} = \begin{cases} x_i & \text{if } (i_1 \dots i_d) \text{ is a permutation of } (\underbrace{i \dots i}_{k} \underbrace{r \dots r}_{d-k}), \\ & \qquad\qquad i = 1, \dots, r-1, \\ t & \text{if } (i_1 \dots i_d) = (r \dots r), \\ 0 & \text{otherwise,} \end{cases}$$

where $x_1, \dots, x_{r-1}$ and t are arbitrary complex numbers. The main result of this section is the following

Theorem 1. *For $\mathcal{A}_k = \{A_{1,k}, A_{2,k}, \dots\}$ as above, the value of the graph function $\mathcal{F}_{\mathcal{A}_k, I_r}$ on any graph G is given by the formula*

$$\mathcal{F}_{\mathcal{A}_k, I_r}(G) = \sum_{|\lambda| \leq n} t^{n-|\lambda|} p_\lambda(x_1, \dots, x_{r-1})\, N_{k,\lambda}(G), \tag{3}$$

where the sum is taken over the set of all partitions λ of weight $|\lambda| \leq n = |V(G)|$.

Proof. We interprete the indices $1, \dots, r$ as colors of the half-edges of G. A product of n components $A_{d_1,k}^{i_1 \dots i_{d_1}} \dots A_{d_n,k}^{i_{m-d_n+1} \dots i_m}$ (where $n = |V(G)|$ and $m = \sum_{j=1}^n d_j = 2|E(G)|$) contributes non-trivially to $\mathcal{F}_{\mathcal{A}_k, I_r}(G)$ if and only if the colors agree on each edge of G or, equivalently, if and only if for each edge the both indices that label two of its half-edges are the same. Thus, in this case the non-zero contributions are in one-to-one correspondence with edge colorings of G in r colors with the following properties:

(i) an edge incident to a vertex of degree $< k$ has color r, and

(ii) at each vertex $v_j \in V(G)$ of degree $d_j \geq k$ exactly k edges incident to it have some color $i_j \in \{1, \dots, r\}$, and the rest $d_i - k$ edges have color r (if an edge makes a loop we count it twice).

The closure of the union of edges with colors $1, \dots, r-1$ is a k-regular subgraph H in G, and every connected component H_j of H is colored in one of the colors $i_j \in \{1, \dots, r-1\}$. The contribution to $\mathcal{F}_{\mathcal{A}_k, I_r}(G)$ from this coloring is $t^{n-|\lambda_H|} \prod_{j=1}^{l(H)} x_{i_j}^{|V(H_j)|}$, where $\lambda_H = [|V(H_1)|, \dots, |V(H_l)|]$ is the partition associated with H and $l = l(H)$ is the number of connected components of H. Therefore, the contribution from all possible colorings of the subgraph H is equal to

$$t^{n-|\lambda_H|} \prod_{j=1}^{l(H)} \left(\sum_{i=1}^{r-1} x_i^{|V(H_j)|} \right) = t^{n-|\lambda_H|} p_{\lambda_H}(x_1, \dots, x_{r-1}),$$

and summig up the contributions from all k-regular subgraphs in G we get the assertion of the theorem. $\square$

Corollary 1. *The graph function $\mathcal{F}_{\mathcal{A}_k, I_r}$, depending on $x_1, \dots, x_{r-1}$ and t as parameters, determines the numbers $N_{k,\lambda}(G)$ uniquely for any graph G with $n \le r-1$ vertices.*

Proof. By Theorem 1, the graph function $\mathcal{F}_{\mathcal{A}_k, I_r}$ with values in $\mathbb{C}$ factors through the ring $\mathbb{C}[x_1, \dots, x_{r-1}]^{S_{r-1}}$ of symmetric polynomials in $r-1$ independent variables $x_1, \dots, x_{r-1}$. It is well known that the polynomials $p_k(x_1, \dots, x_{r-1})$, $k = 1, \dots, n$, are algebraically independent in $\mathbb{C}[x_1, \dots, x_{r-1}]^{S_{r-1}}$ provided $n \le r-1$. Therefore, in this case the graph function $\mathcal{F}_{\mathcal{A}_k, I_r}(G)$ determines the coefficients $N_{k,\lambda}(G)$ in (3) uniquely. □

Remark 1. Since the coefficients $N_{k,\lambda}(G)$ in (3) are *non-negative* integers, we can uniquely find them out when

$$r \ge 1 + \max_{H \subset G} l(H),$$

where $l(H)$ is the number of connected componenets of H and the maximum is taken over all k-regular subgraphs H in G, but we will not dwell on this issue here.

Below are two special cases of Theorem 1 of independent interest.

Corollary 2. *Put $r = 2$, $x_1 = 1$ and $t = 0$. Then for any graph G the value $\mathcal{F}_{\mathcal{A}_k, I_2}(G)$ is the number of* k-factors*, or spanning k-regular subgraphs in G.*

Proof. By Theorem 1,

$$\mathcal{F}_{\mathcal{A}_k, I_2}(G) = x_1^n \sum_{|\lambda| = n} N_{k,\lambda}(G).$$

□

In the simplest case when $k = 1$, Corollary 1 counts the number of 1-factors, or *perfect mathcings* in G.

The next statement concerns *connected* k-factors of G:

Corollary 3. *Put $r = n+1$, $x_j = e^{2\pi\sqrt{-1}j/n}$, $(j = 1, \dots, n)$ and $t = 0$. Then for any graph G the number of connected k-factors in G is equal to $\frac{1}{n}\mathcal{F}_{\mathcal{A}_k, I_{n+1}}(G)$, where n is the number of vertices of G.*

Proof. In this case

$$p_k(x_1, \dots, x_n) = \begin{cases} 0, & k = 1, \dots, n-1, \\ n, & k = n. \end{cases}$$

By Theorem 1 we have

$$\mathcal{F}_{\mathcal{A}_k, I_{n+1}}(G) = n\,,$$

where $[n]$ denotes the 1-element partition of $n = |V(G)|$ (by definition, $N_{k,[n]}(G)$ is the number of connected k-factors). $\square$

4. Computational complexity

The value $\mathcal{F}_{\mathcal{A}_k, I_r}(G)$ can be effectively computed for any graph G as explained in Section 2. In general, this is a hard computational problem. To make things less complicated let us take $r = 2$. Then Corollary 2 provides a relatively simple algorithm for counting the number of k-factors in graphs. (Note that even the case $k = 1$, or enumeration of perfect matchings, is a well-known $\#P$-complete problem.)

The computational complexity of the above algorithm depends on two main points:

(1) the succession of tensor contractions along the edges of G (or simply edge contractions);
(2) the utilization of the special form of tensors $A_{d,k}$;

What concerns the first point, the objective is to choose a sequence of edge contractions that keeps the maximal tensor valency (or vertex degree) as small as possible. This problem was solved in [2]. Take a sequence of edge contractions reducing G to a point. The *complexity* of this sequence is the maximum vertex degree during the contraction process. The *contraction complexity* $cc(G)$ is the minimal complexity over all sequences of edge contractions. A nice result of [2] states that $cc(G) = tw(G^*) + 1$, where G^* is the linear graph of G, and $tw(G^*)$ is the *treewidth* of G^*. Though computing the treewidth of a general graph is NP-hard, a tree decomposition of G^* of width $O(tw(G^*))$ can be obtained in time $|V(G^*)|^{O(1)} \exp(O(tw(G^*))$ [4]. Moreover, given a tree decomposition of G^* of width w, a sequence of edge contractions in G of complexity not greater than $w + 1$ can be found in polynomial time. Thus, the results of [2] give a rough estimate of the computational complexity of our algorithm by $|V(G)|^{O(1)} \exp(O(tw(G^*)))$. So, for graphs whose line graphs have bounded treewidth our algorithm works quite fast. Moreover, known constructions of almost optimal tree-decompositions (cf. [4]) give almost optimal edge contraction sequences.

As for the second point mentioned above, the situation is less clear at the moment. Note that the estimate of [2] is rather general and applies to arbitrary tensor networks. In our case it can be considerably sharper, since the tensor networks we use are of very special types. In particular, Sylvester's theory of decomposing symmetric tensors into

sums of symmetric powers of vectors may appear quite useful in improving the efficiency of our algorithm.[2] However, this is still a work in progress.

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[2]This observation belongs to V. N. Vassiliev.